Bell inequalities stronger than the CHSH inequality for 3-level isotropic states

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We show that some two-party Bell inequalities with two-valued observables are stronger than the CHSH inequality for $3 \otimes 3$ isotropic states in the sense that they are violated by some isotropic states in the $3 \otimes 3$ system that do not violate the CHSH inequality. These Bell inequalities are obtained by applying triangular elimination to the list of known facet inequalities of the cut polytope on nine points. This gives a partial solution to an open problem posed by Collins and Gisin. The results of numerical optimization suggest that they are candidates for being stronger than the I_{3322} Bell inequality for $3 \otimes 3$ isotropic states. On the other hand, we found no Bell inequalities stronger than the CHSH inequality for $2 \otimes 2$ isotropic states. In addition, we illustrate an inclusion relation among some Bell inequalities derived by triangular elimination.

I. INTRODUCTION

Bell inequalities and their violation are an important topic in quantum theory [1, 2]. Pitowsky [3, 4] introduced convex polytopes called *correlation polytopes* which represent the set of possible results of various correlation experiments. A Bell inequality is an inequality valid for a certain correlation polytope. The correlation experiments we consider in this paper are those between two parties, where one party has $m_{\rm A}$ choices of two-valued measurements and the other party has $m_{\rm B}$ choices. The Clauser-Horne-Shimony-Holt inequality [5] is an example of a Bell inequality in this setting with $m_{\rm A}=m_{\rm B}=2$.

Separable states satisfy all Bell inequalities with all measurements by definition. In a seminal paper [6], Werner disproved the converse: there exists a quantum mixed state ρ which is entangled but satisfies all Bell inequalities. To overcome the difficulty of proving these two properties of ρ , he investigated states of very high symmetry now called Werner states. Collins and Gisin [7] compared the strengths of Bell inequalities by introducing a relevance relation between two Bell inequalities, and they showed that a Bell inequality named I_{3322} is relevant to the well-known CHSH inequality. Here relevance means that there is a quantum mixed state ρ such that ρ satisfies the CHSH inequality (with all measurements) but ρ violates the I₃₃₂₂ inequality (with some measurements). The state ρ they found has less symmetry than the Werner states.

A test of relevance is a computationally difficult problem. For one thing, to test relevance, one must tell whether a given state satisfies a given Bell inequality for all measurements or not. This can be cast as a bilinear semidefinite programming problem, which is a hard opti-

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mization problem. The "see-saw iteration" algorithm is used to solve it in literature [1]. Although it is not guaranteed to give the global optimum, multiple runs with different initial solutions seem sufficient for many cases. Another difficulty is to choose the appropriate state ρ . Collins and Gisin overcome this difficulty by restricting states, which we will describe in Section II C.

Collins and Gisin showed numerically that the I₃₃₂₂ Bell inequality is not relevant to the CHSH inequality for 2-level Werner states. They posed an open problem [8]: "Find Bell inequalities which are stronger than the CHSH inequalities in the sense that they are violated by a wider range of Werner states." To answer this problem, we test 89 Bell inequalities for 2- and 3level isotropic states by using the see-saw iteration algorithm. Isotropic states are a generalization of 2-level Werner states in that they are convex combinations of a pure maximally entangled state and the maximally mixed state. The high symmetry of the isotropic states allows us to calculate the maximum violation of the CHSH inequality by 3-level isotropic states analytically. The 89 inequalities used in the test are the Bell inequalities that involve at most five measurements per party in the list of more than 200,000,000 tight Bell inequalities recently obtained by Avis, Imai, Ito and Sasaki [9, 10] by using a method known as triangular elimination. We restrict computation to these 89 inequalities because the optimization problem related to inequalities with many measurements is difficult to solve. As a result, we find five inequalities which are relevant to the CHSH inequality for 3-level isotropic states. They answer Collins and Gisin's problem where Werner states are replaced by 3level isotropic states. We give empirical evidence that the five inequalities are also relevant to the I_{3322} inequality. To the best of our knowledge, no such Bell inequalities were previously known.

The rest of the paper is organized as follows. Section II explains the necessary concepts. Section III discusses inclusion relation, which is used to prove irrelevance of a

Bell inequality to another, and gives. the inclusion relation among the Bell inequalities we used in our experiments. Section IV explains the method and the results of our experiments to test relevance for 2- and 3-level isotropic states. Section V concludes the paper and mentions some open problems.

II. PRELIMINARIES

A. Bell inequalities

We consider the following correlation experiment. Suppose that two parties called Alice and Bob share a quantum state ρ . Alice has $m_{\rm A}$ choices $A_1, \ldots, A_{m_{\rm A}}$ of two-valued measurements and Bob has $m_{\rm B}$ choices $B_1, \ldots, B_{m_{\rm B}}$. We call the two possible outcomes of the measurements 1 and 0. The result of this correlation experiment can be represented by an $(m_{\rm A}+m_{\rm B}+m_{\rm A}m_{\rm B})$ -dimensional vector \boldsymbol{q} , where for $1 \leq i \leq m_{\rm A}$ and $1 \leq j \leq m_{\rm B}$, the variables q_{i0} , q_{0j} and q_{ij} represent the probability that the outcome of A_i is 1, that the outcome of B_j is 1, and that two outcomes of both A_i and B_j are 1, respectively.

An inequality $\mathbf{a}^{\mathrm{T}}\mathbf{q} \leq a_0$, where \mathbf{a} is an $(m_{\mathrm{A}} + m_{\mathrm{B}} + m_{\mathrm{A}}m_{\mathrm{B}})$ -dimensional vector and a_0 is a scalar, is called a *Bell inequality* if it is satisfied for all separable states ρ and all choices of measurements $A_1, \ldots, A_{m_{\mathrm{A}}}$, $B_1, \ldots, B_{m_{\mathrm{B}}}$. The nontrivial Bell inequality with the smallest values of m_{A} and m_{B} is the CHSH inequality [5]

$$-q_{10} - q_{01} + q_{11} + q_{21} + q_{12} - q_{22} \le 0 \tag{1}$$

for $m_{\rm A} = m_{\rm B} = 2$.

A Bell inequality is said to be *tight* if it cannot be written as a positive sum of two different Bell inequalities. The CHSH inequality is an example of a tight Bell inequality. Tight Bell inequalities are more useful as a test of the nonlocality than the other Bell inequalities, since if a state violates a non-tight Bell inequality $\mathbf{a}^{\mathrm{T}}\mathbf{q} \leq a_0$, then the same state violates one of tight Bell inequalities which sum up to $\mathbf{a}^{\mathrm{T}}\mathbf{q} \leq a_0$.

Throughout this paper, we denote a Bell inequality $a^{T}q \leq a_0$ by

$$\begin{pmatrix}
 & | | (A_1) & \cdots & (A_{m_A}) \\
 & | | a_{10} & \cdots & a_{m_A0} \\
\hline
(B_1) & a_{01} & | | a_{11} & \cdots & a_{m_A1} \\
 & \vdots & \vdots & \vdots & & \vdots \\
 & (B_{m_B}) & a_{0m_B} & | | a_{1m_B} & \cdots & a_{m_Am_B} \\
\end{pmatrix} \le a_0,$$

following the notation by Collins and Gisin used in [7] (with labels added to indicate which rows and columns correspond to which measurements). For example, the

CHSH inequality (1) is written as

$$\begin{pmatrix}
 & | (A_1) & (A_2) \\
 & | -1 & 0 \\
\hline
 & (B_1) & -1 & 1 & 1 \\
 & (B_2) & 0 & 1 & -1
\end{pmatrix} \le 0.$$

Another Bell inequality found by Pitowsky and Svozil [11] and named I_{3322} inequality by Collins and Gisin [7] is written as

$$\begin{pmatrix}
 & | (A_1) & (A_2) & (A_3) \\
\hline
 & | -1 & 0 & 0 \\
\hline
 & | (B_1) & -2 & 1 & 1 & 1 \\
 & | (B_2) & -1 & 1 & 1 & -1 \\
 & | (B_3) & 0 & 1 & -1 & 0
\end{pmatrix} \le 0.$$
(2)

Recently Avis, Imai, Ito and Sasaki [9, 10] proposed a method known as triangular elimination that can be used to generate tight Bell inequalities from known tight inequalities for a well-studied related polytope, known as the cut polytope. They obtained a list of more than 200,000,000 tight Bell inequalities by applying triangular elimination to a list [12] of tight inequalities for the cut polytope on 9 points, CUT_9^{\square} . There are 89 Bell inequalities which involve five measurements per party in the list, and they are used in this paper. Among them are the CHSH inequality, the positive probability (trivial) inequality, the I_{mm22} inequalities for m=3,4,5, the $I_{3422}^{(2)}$ inequality [7] and other unnamed Bell inequalities. We label the 89 inequalities as A1 to A89. The list of these inequalities is available online [13].

B. Violation of a Bell inequality and bilinear semidefinite programming

A test whether there exists a set of measurements violating a given Bell inequality in a given state can be cast as a bilinear semidefinite programming problem as follows. Let ρ be a density matrix in the $d\otimes d$ system and $\mathbf{a}^T\mathbf{q}\leq a_0$ be a Bell inequality. Each measurement by Alice is represented by a positive operator valued measure (POVM) $(E_i, I-E_i)$, where E_i is a Hermitian $d\times d$ matrix such that both E_i and $I-E_i$ are nonnegative definite and I is the identity matrix of size $d\times d$. Similarly, each measurement by Bob is represented by a POVM $(F_j, I-F_j)$. For concise notation, we let $E_0=F_0=I$. Then the test whether there exists a set of violating measurements or not can be formulated as:

$$\max \sum_{\substack{0 \le i \le m_{\mathrm{A}} \\ 0 \le j \le m_{\mathrm{B}} \\ (i,j) \ne (0,0)}} a_{ij} \operatorname{tr}(\rho(E_i \otimes F_j)) - a_0 \tag{3}$$

where
$$E_0 = F_0 = I$$
, $\overline{E_i}^{\mathrm{T}} = E_i$, $\overline{F_j}^{\mathrm{T}} = F_j$, $O \leq E_i, F_j \leq I$.

Here the notation $X \leq Y$ means that Y - X is nonnegative definite. The optimal value of (3) is positive if and only if there exist violating measurements, and if so, the optimal solution gives the set of measurements that is maximally violating the given Bell inequality in the given state. If we fix one of the two groups of variables $\{E_1, \ldots, E_{m_A}\}$ and $\{F_1, \ldots, F_{m_B}\}$, (3) becomes a semidefinite programming problem on the other group of variables. In this respect, (3) can be seen as a variation of bilinear programming [14] with semidefinite constraints. The optimization problem (3) is NP-hard, even for the case d=1, as follows from results in [15, Sections 5.1, 5.2].

If d=2 and the inequality $\mathbf{a}^{\mathrm{T}}\mathbf{q} \leq a_0$ is the CHSH inequality, then (3) can be solved analytically [16], hence the Horodecki criterion, a necessary and sufficient condition for a state ρ in the $2 \otimes 2$ system to satisfy the CHSH inequality for all measurements. However, in general, the analytical solution of (3) is not known. This seems natural, given the difficulty of bilinear programming. Section 2 of [14] describes a hill-climbing algorithm which computes a local optimum by fixing one of the two groups of variables and solving the subproblem to optimize variables in the other groups repeatedly, exchanging the role of the two groups in turn. "See-saw iteration" [1] uses the same method combined with the observation that in the case of (3), each subproblem can be solved efficiently by just computing the eigenvectors of a Hermitian $d \times d$ matrix.

There exists a set of projective measurements $E_1, \ldots, E_{m_{\rm A}}$ and $F_1, \ldots, F_{m_{\rm B}}$ which attains the maximum of (3). This fact is obtained from the proof of Theorem 5.4 in [17] by Cleve, Høyer, Toner and Watrous. Though they prove the case where ρ is also variable, the relevant part in the proof is true even if the state is fixed. See-saw iteration always produces projective measurements as a candidate for the optimal measurements.

C. Relevance relation

Collins and Gisin [7] introduced the notion of relevance between two Bell inequalities and showed that the Bell inequality (2) named I_{3322} is relevant to the well-known CHSH inequality. Here relevance means that there is a quantum mixed state ρ such that ρ satisfies the CHSH inequality (with any measurements) but ρ violates the I_{3322} inequality (with some measurements). They prove the relevance of the I_{3322} inequality to the CHSH inequality by giving an explicit example of a state ρ in the $2 \otimes 2$ system which satisfies the CHSH inequality for all measurements, and which violates the I_{3322} inequality for certain measurements.

Part of the difficulty of testing relevance comes from how to choose an appropriate state ρ . Even if we only consider the $2 \otimes 2$ system, the space of mixed states is 15dimensional. Collins and Gisin overcome this difficulty by restricting the states to those parameterized by two variables θ and α : $\rho(\theta,\alpha) = \alpha|\varphi_{\theta}\rangle\langle\varphi_{\theta}| + (1-\alpha)|01\rangle\langle01|$, where $|\varphi_{\theta}\rangle = \cos\theta|00\rangle + \sin\theta|11\rangle$. For any θ , the variable α can be maximized by using the Horodecki criterion [16] to give a state $\rho(\theta,\alpha_{\rm max})$ on the boundary of the set of the states which satisfy the CHSH inequality for all measurements. Then they compute the maximum violation of the I_{3322} inequality by $\rho(\theta,\alpha_{\rm max})$ for various values of θ , and find a state satisfying the CHSH inequality but not the I_{3322} inequality.

III. INCLUSION RELATION

Before discussing relevance relations among Bell inequalities for isotropic states, we need an introduction to inclusion relation among these inequalities, which is used to distinguish "obvious" relevance relations from the other relevance relations.

A. Definition of inclusion relation

Collins and Gisin [7] pointed out that the CHSH inequality is irrelevant to the I_{3322} inequality since if we pick the I_{3322} inequality and fix two measurements A_3 and B_1 to the deterministic measurement whose result is always 0, the inequality becomes the CHSH inequality. Generalizing this argument, Avis, Imai, Ito and Sasaki [10] introduced the notion of inclusion relation between two Bell inequalities. A Bell inequality $\boldsymbol{a}^T\boldsymbol{q} \leq 0$ includes another Bell inequality $\boldsymbol{b}^T\boldsymbol{q} \leq 0$ if we can obtain the inequality $\boldsymbol{b}^T\boldsymbol{q} \leq 0$ by fixing some measurements in the inequality $\boldsymbol{a}^T\boldsymbol{q} \leq 0$ to deterministic ones (i.e. measurements whose result is always 1 or always 0).

Here we give a formal definition of the inclusion relation. Let $\mathbf{a}^{\mathrm{T}}\mathbf{q} \leq 0$ be a Bell inequality with $m_A + m_B$ measurements and $\mathbf{b}^{\mathrm{T}}\mathbf{q} \leq 0$ another with $n_A + n_B$ measurements, and assume $m_A \geq n_A$ and $m_B \geq n_B$. The inequality $\mathbf{a}^{\mathrm{T}}\mathbf{q} \leq 0$ includes $\mathbf{b}^{\mathrm{T}}\mathbf{q} \leq 0$ if there exists a Bell inequality $(\mathbf{a}')^{\mathrm{T}}\mathbf{q} \leq 0$ equivalent to the inequality $\mathbf{a}^{\mathrm{T}}\mathbf{q} \leq 0$ such that $a'_{ij} = b_{ij}$ for any $0 \leq i \leq n_A$ and any $0 \leq j \leq n_B$. Here equivalence means that the inequality $(\mathbf{a}')^{\mathrm{T}}\mathbf{q} \leq 0$ can be obtained from another $\mathbf{a}^{\mathrm{T}}\mathbf{q} \leq 0$ by zero or more applications of party exchange, observable exchange and value exchange. See e.g. [18] or [7] for more about equivalence of Bell inequalities. Readers familiar with the cut polytope will recognize that inclusion is a special case of collapsing [15, Section 26.4].

By using this notion, a Bell inequality $\boldsymbol{a}^{\mathrm{T}}\boldsymbol{q} \leq 0$ is irrelevant to another Bell inequality $\boldsymbol{b}^{\mathrm{T}}\boldsymbol{q} \leq 0$ if the inequality $\boldsymbol{b}^{\mathrm{T}}\boldsymbol{q} \leq 0$ includes the inequality $\boldsymbol{a}^{\mathrm{T}}\boldsymbol{q} \leq 0$.

B. Inclusion relation between known Bell inequalities with at most 5 measurements per party

We tested the inclusion relation among the 89 tight Bell inequalities described in Section II A. Figure 1 on the last page shows the result. In the figure, the serial number of each inequality is shown with the number of measurements (omitted for inequalities with 5+5 measurements) and its name (if there is one). An arc from one inequality to another means that the former includes the latter. Since the inclusion relation is transitive, the arcs which are derived by other arcs are omitted. An asterisk (*) on the right of the serial number indicates the inequality is a candidate for being relevant to I_{3322} . Relevancy was tested empirically using the method described in Section IV C.

From the figure, one might be tempted to conjecture that the CHSH inequality is included in all tight Bell inequalities other than the positive probability inequality. However, this is not true. Enumeration of tight Bell inequalities with four measurements by each party using the general convex hull computation package lrs [19] takes an unrealistically long time, but in a partial list, we have some counterexamples. In the notation by Collins and Gisin, they are:

IV. RELEVANCE FOR 2- AND 3-LEVEL ISOTROPIC STATES

A. Violation of a Bell inequality by isotropic states

Let $|\psi_d\rangle$ be a maximally entangled state in $d\otimes d$ system:

$$|\psi_d\rangle = \frac{1}{\sqrt{d}}(|00\rangle + |11\rangle + \dots + |d-1, d-1\rangle).$$

The d-level isotropic state [20] (or $U \otimes U^*$ -invariant state [21]) $\rho_d(\alpha)$ of parameter $0 \le \alpha \le 1$ is a state defined by:

$$\rho_d(\alpha) = \alpha |\psi_d\rangle \langle \psi_d| + (1 - \alpha) \frac{I}{d^2}$$

$$= \frac{\alpha}{d} (|00\rangle + |11\rangle + \dots + |d - 1, d - 1\rangle)$$

$$(\langle 00| + \langle 11| + \dots + \langle d - 1, d - 1|) + \frac{1 - \alpha}{d^2} I.$$

With $\alpha=0$, $\rho_d(\alpha)$ is a maximally mixed state I/d^2 , which is separable and therefore satisfies all the Bell inequalities for all measurements. More generally, it is known that $\rho_d(\alpha)$ is separable if and only if $\alpha \leq 1/(d+1)$ [21]. With $\alpha=1$, $\rho_d(\alpha)$ is a maximally entangled state $|\psi_d\rangle\langle\psi_d|$. Therefore $\rho_d(\alpha)$ represents a state in the middle between a separable state and a maximally entangled state for general α .

If two states ρ and ρ' satisfy a Bell inequality for all measurements, then their convex combination $t\rho + (1-t)\rho'$ also satisfies the same Bell inequality for all measurements. This means that for any $d \geq 2$ and any Bell inequality $\boldsymbol{a}^{\mathrm{T}}\boldsymbol{q} \leq 0$, there exists a real number $0 \leq \alpha_{\mathrm{max}} \leq 1$ such that $\rho_d(\alpha)$ satisfies the inequality $\boldsymbol{a}^{\mathrm{T}}\boldsymbol{q} \leq 0$ for all measurements if and only if $\alpha \leq \alpha_{\mathrm{max}}$. A smaller value of α_{max} means that the Bell inequality is more sensitive for isotropic states.

B. Violation of the CHSH inequality by 3-level isotropic states

In this section, we prove that the maximum violation of the CHSH inequality by the 3-level isotropic state $\rho_3(\alpha)$ is given by $\max\{0, \alpha(3\sqrt{2}+1)/9-4/9\}$. As a corollary, the threshold α_{\max} for the CHSH inequality with d=3 is equal to $\alpha_{\max}=4/(3\sqrt{2}+1)=0.76297427932$.

As we noted in Section IIB, we can restrict E_1 , E_2 , F_1 and F_2 to projective measurements in the optimization problem (3). We consider the rank of measurements E_1 , E_2 , F_1 and F_2 . Since the CHSH inequality is not violated if any one of E_1 , E_2 , F_1 and F_2 has rank zero or three, we only need to consider the case where the four measurements E_1 , E_2 , F_1 and F_2 have rank one or two. Instead of considering all the combinations of ranks of the measurements, we fix their rank to one and consider the inequalities obtained by exchanging outcomes "0" and "1" of some measurements in the CHSH inequality. (In terms of the cut polytope, this transformation corresponds to switching [15, Section 26.3] of inequalities. See [10] for details.) For example, suppose that E_1 and F_1 have rank two and E_2 and F_2 have rank one in the optimal set of measurements. Then instead of the CHSH inequality in the form (1), we exchange the two outcomes of measurements E_1 and F_1 in the inequality, and obtain (in the Collins-Gisin notation):

$$\left(\begin{array}{c|cc} & (A_1) & (A_2) \\ \hline & 0 & 1 \\ \hline (B_1) & 0 & 1 & -1 \\ (B_2) & 1 & -1 & -1 \end{array}\right) \le 1, \tag{4}$$

with the four measurements of rank one. We have $2^4 = 16$ possibilities for the ranks of the four measurements and corresponding 16 inequalities transformed from (1). These inequalities are identical to either (1) or (4) if it is relabelled appropriately. Therefore, we can assume

the four measurements have rank one at the expense of considering the inequality (4) in addition to (1).

We compute the maximum violation $V(\alpha)$ (resp. $V'(\alpha)$) of the inequality (1) (resp. (4)) under the assumption that the four measurements have rank one. In the maximally mixed state $\rho_3(0) = I_9/9$, the violations of the two inequalities are constant regardless of the actual measurements, and they are:

$$V(0) = -q_{10} - q_{01} + q_{11} + q_{12} + q_{21} - q_{22}$$

= -1/3 - 1/3 + 1/9 + 1/9 + 1/9 - 1/9 = -4/9,
$$V'(0) = q_{20} + q_{02} + q_{11} - q_{12} - q_{21} - q_{22} - 1$$

= 1/3 + 1/3 + 1/9 - 1/9 - 1/9 - 1/9 - 1 = -5/9.

Since the violations of the inequalities are constant in the state $\rho_3(0)$, the maximum violation in the state $\rho_3(\alpha)$ is achieved by the optimal set of measurements in the state $\rho_3(1)$, $V(\alpha) = \alpha V(1) + (1 - \alpha)V(0)$ and $V'(\alpha) = \alpha V'(1) + (1 - \alpha)V'(0)$. Therefore, what remains is to compute the values of V(1) and V'(1).

To obtain the value of V(1), let $E_i = |\varphi_{1i}\rangle\langle\varphi_{1i}|$, $F_j = |\varphi_{2j}\rangle\langle\varphi_{2j}|$, $|\varphi_{1i}\rangle = x_{i0}|0\rangle + x_{i1}|1\rangle + x_{i2}|2\rangle$ and $|\varphi_{2j}\rangle = \overline{y_{j0}}|0\rangle + \overline{y_{j1}}|1\rangle + \overline{y_{j2}}|2\rangle$. Note that \boldsymbol{x}_1 , \boldsymbol{x}_2 , \boldsymbol{y}_1 and \boldsymbol{y}_2 are unit vectors in \mathbb{C}^3 . Using them, the violations of the inequality (1) is equal to

$$-\frac{2}{3} + \frac{1}{3}(|\boldsymbol{x}_1 \cdot \boldsymbol{y}_1|^2 + |\boldsymbol{x}_1 \cdot \boldsymbol{y}_2|^2 + |\boldsymbol{x}_2 \cdot \boldsymbol{y}_1|^2 - |\boldsymbol{x}_2 \cdot \boldsymbol{y}_2|^2), (5)$$

If we fix y_1 and y_2 arbitrarily, then optimization of x_1 and x_2 in (5) can be performed separately. Since (5) depends only on the inner products of the vectors and not the vectors themselves, we can replace the vectors x_1 and x_2 with their projection onto the subspace spanned by y_1 and y_2 . This means that we can consider the four vectors x_1 , x_2 , y_1 and y_2 are vectors in \mathbb{C}^2 whose lengths are at most one. Then the Tsirelson inequality [22, 23] tells the maximum of $|x_1 \cdot y_1|^2 + |x_1 \cdot y_2|^2 + |x_2 \cdot y_1|^2 - |x_2 \cdot y_2|^2$ is equal to $\sqrt{2} + 1$, and the vectors giving this maximum are $|\varphi_{11}\rangle = \cos(\pi/4)|0\rangle + \sin(\pi/4)|1\rangle$, $|\varphi_{12}\rangle = |0\rangle$, $|\varphi_{21}\rangle = \cos(\pi/8)|0\rangle + \sin(\pi/8)|1\rangle$ and $|\varphi_{22}\rangle = \cos(3\pi/8)|0\rangle + \sin(3\pi/8)|1\rangle$. The violation of (1) is $V(1) = (\sqrt{2} - 1)/3 = 0.138071$, and $V(\alpha) = (1 - \alpha)(-4/9) + \alpha(\sqrt{2} - 1)/3 = \alpha(3\sqrt{2} + 1)/9 - 4/9$.

By a similar argument, we can compute the value of V'(1). Using the same definition for x_1 , x_2 , y_1 and y_2 , the violation of the inequality (4) is given by

$$-\frac{4}{3} + \frac{1}{3}(|\boldsymbol{x}_1 \cdot \boldsymbol{y}_1|^2 - |\boldsymbol{x}_1 \cdot \boldsymbol{y}_2|^2 - |\boldsymbol{x}_2 \cdot \boldsymbol{y}_1|^2 - |\boldsymbol{x}_2 \cdot \boldsymbol{y}_2|^2).$$
(6)

The maximum of (6) is equal to -1, and it is achieved by setting $|\varphi_{11}\rangle = |\varphi_{21}\rangle = |0\rangle$, $|\varphi_{12}\rangle = |1\rangle$ and $|\varphi_{22}\rangle = |2\rangle$. Therefore V'(1) = -1 and $V'(\alpha) = -14\alpha/9 - 5/9 < 0$. This means the inequality (4) is never violated under the assumption that the four measurements have rank one.

Removing the assumption of the ranks of the measurements, we obtain that the maximum violation of the CHSH inequality in the state $\rho_3(\alpha)$ is given by $\max\{0, V(\alpha), V'(\alpha)\} = \max\{0, \alpha(3\sqrt{2}+1)/9 - 4/9\}.$

C. Computation of violation of Bell inequalities with at most 5 measurements per party

We performed preliminary experiments to compute an upper bound on the value of α_{max} with d=2 and d=3for the 89 inequalities described in Section IIA. The see-saw iteration algorithm finds a candidate for the optimal solution of (3). When $0 \le \alpha \le 1$ is given, we can use this search algorithm to tell whether $\alpha_{\rm max} < \alpha$ (if violating measurements are found) or $\alpha_{\text{max}} \geq \alpha$ (otherwise), if we ignore the possibility that the hill-climbing search fails to find the global optimum. This allows us to compute the value of α_{max} by binary search. In reality, the hill-climbing search sometimes fails to find the global optimum, and if it finds violating measurements then it surely means $\alpha_{\rm max} < \alpha$, whereas if it does not find violating measurements then it does not necessarily mean $\alpha_{\rm max} \geq \alpha$. Therefore, the value given by binary search is not necessarily the true value of α_{max} but an upper bound on it.

In each step of the binary search, we performed a see-saw iteration with 1,000 random initial measurements and picked the solution giving the maximum in the 1,000 trials. To compute eigenvalues and eigenvectors of 3×3 Hermitian matrix, we used LAPACK [24] with ATLAS [25, 26]. All computations were performed using double-precision floating arithmetic. Due to numerical error, the computation indicates a small positive violation even if the state does not violate the inequality. Therefore, we only consider violation greater than 10^{-13} significant.

For d=2, the computation gave an upper bound 0.70711 for all inequalities except for the positive probability inequality. (For the positive probability inequality we have $\alpha_{\rm max}=1$ since it is satisfied by any quantum state.) It is known that in the case d=2, the CHSH inequality is satisfied if and only if $\alpha \leq 1/\sqrt{2}=0.70711$ from the Horodecki criterion [16]. These results suggest that there may not be any Bell inequalities relevant to the CHSH inequality for 2-level isotropic states, indicating the negative answer to Gisin's problem [8] in the case of 2-level system.

We performed the same computation for d=3. This time some Bell inequalities gave a smaller value of $\alpha_{\rm max}$ than the CHSH inequality did. Some of them gave a small value of $\alpha_{\rm max}$ simply because it includes another such inequality. Filtering them out, we identified five inequalities which are candidates for being relevant to the CHSH inequality for the 3-level isotropic states. Rows and columns in bold font indicate that they correspond to nodes added by triangular elimination.

$\alpha_{ m max}$	Bell inequality	Original cut polytope inequality
0.7447198434	A28	7
0.7453308276	A27	6
0.7553800191	A5	8 (Par(7), parachute ineq.)
0.7557816805	A56	89
0.7614396336	A8	2 (Pentagonal ineq.)
0.7629742793	A3 (I_{3322})	2 (Pentagonal ineq.)
0.7629742793	A2 (CHSH)	1 (Triangle ineq.)
1	A1 (Positive probability)	1 (Triangle ineq.)

TABLE I: Upper bound of the value of α_{max} obtained by the experiments.

Adding the CHSH and the I_{3322} inequalities, we performed the experiments with 50,000 initial solutions with the seven inequalities. Table I summarizes the results we obtained. In Table I, the column labeled "Original cut polytope inequality" shows the facet inequality of CUT_0^{\sqcup} to which triangular elimination is applied. The number corresponds to the serial number of the facet in cut9.gz of [12]. For the CHSH inequality, the obtained upper bound 0.76298 is consistent with the theoretical value $4/(3\sqrt{2}+1) = 0.762974$ proved in Section IVB. The I₃₃₂₂ inequality gave the same upper bound as the CHSH inequality. Besides, in the optimal measurements with α near $4/(3\sqrt{2}+1)$, the matrices E_3 and F_1 are zero, corresponding to the fact that the I_{3322} inequality includes the CHSH inequality. This is consistent with Collins and Gisin's observation [7] in the $2 \otimes 2$ system that the I_{3322} inequality is not better than the CHSH inequality for states with high symmetry.

Five Bell inequalities A28, A27, A5, A56 and A8 gave a smaller value of $\alpha_{\rm max}$ than $4/(3\sqrt{2}+1)$. The set of measurements giving optimal violation for these Bell inequalities with α slightly larger than the computed value of $\alpha_{\rm max}$ is given in the Appendix.

These Bell inequalities are relevant to the CHSH inequality. As a result, Bell inequalities including any of them are also relevant to the CHSH inequality. Moreover, if the true value of $\alpha_{\rm max}$ for the I₃₃₂₂ inequality is $4/(3\sqrt{2}+1)$, then these five Bell inequalities are also relevant to the I₃₃₂₂ inequality. We make the following conjecture.

Conjecture 1. The state $\rho_3(4/(3\sqrt{2}+1))$ satisfies the I_{3322} inequality for all measurements. In other words, $\alpha_{\max} = 4/(3\sqrt{2}+1)$ for the I_{3322} inequality in the case of d=3.

To support this conjecture, we searched for the optimal measurements for the I_{3322} inequality in the states $\rho_3(\alpha)$ with $\alpha=\alpha_+=0.7629742794>4/(3\sqrt{2}+1)$ and $\alpha=\alpha_-=0.7629742793<4/(3\sqrt{2}+1)$, using see-saw iteration algorithm with random initial solutions. With $\alpha=\alpha_+$, 100 out of 633 trials gave a violation greater than 10^{-13} , whereas with $\alpha=\alpha_-$, none of 50,000 trials gave a violation greater than 3×10^{-15} . Considering numerical error in computation, we consider that this result

can be seen as an evidence that the I_{3322} inequality behaves differently in the state $\rho_3(\alpha)$ depending on whether α is greater or less than $4/(3\sqrt{2}+1)$.

V. CONCLUDING REMARKS

We used numerical optimization to show that certain Bell inequalities are relevant to the CHSH inequality for isotropic states. No Bell inequalities relevant to the CHSH inequality were found for 2-level isotropic states. This supports Collins and Gisin's conjecture in [7] that no such Bell inequalities exist. For 3-level isotropic states, however, five Bell inequalities relevant to the CHSH inequality were found. The results of numerical experiments were given to support the conjecture that they are also relevant for the I₃₃₂₂ inequality.

The violation of the CHSH inequality by 3-level isotropic states was shown by using Tsirelson's inequality. Cleve, Høyer, Toner and Watrous [17] generalize

Tsirelson's inequality to Bell inequalities corresponding to "XOR games," which do not depend on individual variables q_{i0},q_{0j},q_{ij} but only involves combinations in the form $x_{ij}=q_{i0}+q_{0j}-2q_{ij}$. Unfortunately, the I_{3322} inequality is not such an inequality, and we cannot use the result there to prove the theoretical value of $\alpha_{\rm max}$ for the I_{3322} inequality. Among the five Bell inequalities relevant to the CHSH inequality for 3-level isotropic states, the inequality A8, which can be written as $-\sum_{i=1,2}\sum_{j=1,2,3}x_{ij}+x_{13}-x_{23}+x_{14}-x_{34}+x_{25}-x_{35}+x_{41}-x_{42}\leq 0$, is the only one that corresponds to an XOR game. An important open problem is to generalize Cleve, Høyer, Toner and Watrous's result to cover Bell inequalities which do not correspond to XOR games.

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APPENDIX A: OPTIMAL MEASUREMENTS COMPUTED FOR EACH INEQUALITIES

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A28:
                   E_1 = I - |\varphi_{11}\rangle\langle\varphi_{11}|,
                                                                           |\varphi_{11}\rangle = 0.819512|0\rangle + (-0.181891 - 0.067213i)|1\rangle + (0.239561 + 0.483124i)|2\rangle,
                   E_2 = |\varphi_{12}\rangle\langle\varphi_{12}|,
                                                                           |\varphi_{12}\rangle = 0.391928|0\rangle + (0.546808 - 0.330668i)|1\rangle + (-0.064601 + 0.658695i)|2\rangle,
                   E_3 = |\varphi_{13}\rangle\langle\varphi_{13}|,
                                                                           |\varphi_{13}\rangle = 0.585206|0\rangle + (0.266618 - 0.150612i)|1\rangle + (0.721307 - 0.208519i)|2\rangle,
                                                                           |\varphi_{14}\rangle = 0.696701|0\rangle + (0.109760 + 0.562926i)|1\rangle + (0.269399 - 0.336302i)|2\rangle,
                   E_4 = |\varphi_{14}\rangle\langle\varphi_{14}|,
                   E_5 = I - |\varphi_{15}\rangle\langle\varphi_{15}|,
                                                                           |\varphi_{15}\rangle = 0.745551|0\rangle + (0.060720 - 0.038486i)|1\rangle + (0.610743 + 0.256863i)|2\rangle,
                   F_1 = I - |\varphi_{21}\rangle\langle\varphi_{21}|,
                                                                           |\varphi_{21}\rangle = 0.665942|0\rangle + (0.124951 + 0.288249i)|1\rangle + (0.306094 - 0.603430i)|2\rangle,
                   F_2 = I - |\varphi_{22}\rangle\langle\varphi_{22}|,
                                                                           |\varphi_{22}\rangle = 0.794583|0\rangle + (-0.503910 - 0.071325i)|1\rangle + (-0.075809 - 0.322300i)|2\rangle,
                   F_3 = I - |\varphi_{23}\rangle\langle\varphi_{23}|,
                                                                           |\varphi_{23}\rangle = 0.738612|0\rangle + (0.143632 - 0.211840i)|1\rangle + (0.594179 + 0.189467i)|2\rangle,
                   F_4 = |\varphi_{24}\rangle\langle\varphi_{24}|,
                                                                           |\varphi_{24}\rangle = 0.314299|0\rangle + (0.087381 + 0.592536i)|1\rangle + (0.427166 + 0.600009i)|2\rangle,
                   F_5 = I - |\varphi_{25}\rangle\langle\varphi_{25}|,
                                                                           |\varphi_{25}\rangle = 0.745551|0\rangle + (0.060720 + 0.038486i)|1\rangle + (0.610743 - 0.256863i)|2\rangle
A27:
                   E_1 = |\varphi_{11}\rangle\langle\varphi_{11}|,
                                                                           |\varphi_{11}\rangle = 0.512740|0\rangle + (0.141298 - 0.367921i)|1\rangle + (0.118341 - 0.753500i)|2\rangle,
                   E_2 = I - |\varphi_{12}\rangle\langle\varphi_{12}|,
                                                                           |\varphi_{12}\rangle = 0.429346|0\rangle + (0.490358 + 0.190555i)|1\rangle + (-0.588595 - 0.438697i)|2\rangle,
                   E_3 = I - |\varphi_{13}\rangle\langle\varphi_{13}|,
                                                                           |\varphi_{13}\rangle = 0.649098|0\rangle + (-0.034498 + 0.390106i)|1\rangle + (0.648622 + 0.067734i)|2\rangle,
                                                                           |\varphi_{14}\rangle = 0.782874|0\rangle + (-0.199336 - 0.104823i)|1\rangle + (-0.579621 + 0.020651i)|2\rangle,
                   E_4 = |\varphi_{14}\rangle\langle\varphi_{14}|,
                   E_5 = |\varphi_{15}\rangle\langle\varphi_{15}|,
                                                                           |\varphi_{15}\rangle = 0.504711|0\rangle + (0.266955 - 0.029362i)|1\rangle + (-0.176172 - 0.801313i)|2\rangle,
                   F_1 = |\varphi_{21}\rangle\langle\varphi_{21}|,
                                                                           |\varphi_{21}\rangle = 0.477430|0\rangle + (-0.243408 + 0.631106i)|1\rangle + (-0.024181 + 0.560297i)|2\rangle,
                   F_2 = |\varphi_{22}\rangle\langle\varphi_{22}|,
                                                                           |\varphi_{22}\rangle = 0.521997|0\rangle + (0.270933 - 0.132987i)|1\rangle + (0.586914 + 0.540334i)|2\rangle,
                                                                           |\varphi_{23}\rangle = 0.631718|0\rangle + (0.176373 + 0.079451i)|1\rangle + (-0.678537 + 0.321093i)|2\rangle,
                   F_3 = |\varphi_{23}\rangle\langle\varphi_{23}|,
                                                                           |\varphi_{24}\rangle = 0.839814|0\rangle + (-0.361305 - 0.101706i)|1\rangle + (-0.207777 - 0.332648i)|2\rangle,
                   F_4 = |\varphi_{24}\rangle\langle\varphi_{24}|,
                   F_5 = |\varphi_{25}\rangle\langle\varphi_{25}|,
                                                                           |\varphi_{25}\rangle = 0.634648|0\rangle + (-0.135288 + 0.308277i)|1\rangle + (-0.492423 + 0.491328i)|2\rangle
A5:
                                                                           |\varphi_{11}\rangle = 0.079911|0\rangle + (0.347597 - 0.352563i)|1\rangle + (0.852394 + 0.148034i)|2\rangle,
                   E_1 = I - |\varphi_{11}\rangle\langle\varphi_{11}|,
                   E_2 = |\varphi_{12}\rangle\langle\varphi_{12}|,
                                                                           |\varphi_{12}\rangle = 0.466812|0\rangle + (0.336458 - 0.338316i)|1\rangle + (0.063365 - 0.741896i)|2\rangle,
                   E_3 = I - |\varphi_{13}\rangle\langle\varphi_{13}|,
                                                                           |\varphi_{13}\rangle = 0.700997|0\rangle + (-0.090375 + 0.325520i)|1\rangle + (0.625759 - 0.053829i)|2\rangle,
                                                                           |\varphi_{14}\rangle = 0.569742|0\rangle + (-0.703808 - 0.061209i)|1\rangle + (-0.405767 - 0.107957i)|2\rangle,
                   E_4 = |\varphi_{14}\rangle\langle\varphi_{14}|,
                   F_1 = |\varphi_{21}\rangle\langle\varphi_{21}|,
                                                                           |\varphi_{21}\rangle = 0.611974|0\rangle + (0.261472 + 0.553836i)|1\rangle + (-0.402289 + 0.297574i)|2\rangle,
                   F_2 = |\varphi_{22}\rangle\langle\varphi_{22}|,
                                                                           |\varphi_{22}\rangle = 0.743739|0\rangle + (-0.644052 - 0.121119i)|1\rangle + (-0.050055 - 0.121959i)|2\rangle,
                   F_3 = |\varphi_{23}\rangle\langle\varphi_{23}|,
                                                                           |\varphi_{23}\rangle = 0.327181|0\rangle + (-0.492820 + 0.363796i)|1\rangle + (-0.442899 + 0.567075i)|2\rangle,
                   F_4 = I - |\varphi_{24}\rangle\langle\varphi_{24}|,
                                                                           |\varphi_{24}\rangle = 0.558366|0\rangle + (0.295353 - 0.157594i)|1\rangle + (0.593099 + 0.473699i)|2\rangle
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A56:

A8:

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E_1 = |\varphi_{11}\rangle\langle\varphi_{11}|,
                                                        |\varphi_{11}\rangle = 0.764669|0\rangle + (0.520735 - 0.023147i)|1\rangle + (0.314448 - 0.211429i)|2\rangle,
E_2 = I - |\varphi_{12}\rangle\langle\varphi_{12}|,
                                                        |\varphi_{12}\rangle = 0.523087|0\rangle + (-0.660068 + 0.130414i)|1\rangle + (0.115043 + 0.510340i)|2\rangle,
E_3 = I - |\varphi_{13}\rangle\langle\varphi_{13}|,
                                                        |\varphi_{13}\rangle = 0.651881|0\rangle + (0.010176 - 0.025750i)|1\rangle + (-0.599260 + 0.463866i)|2\rangle,
E_4 = I - |\varphi_{14}\rangle\langle\varphi_{14}|,
                                                        |\varphi_{14}\rangle = 0.480244|0\rangle + (0.435821 - 0.476742i)|1\rangle + (0.370530 + 0.463520i)|2\rangle,
E_5 = I - |\varphi_{15}\rangle\langle\varphi_{15}|,
                                                        |\varphi_{15}\rangle = 0.484893|0\rangle + (0.214118 + 0.403736i)|1\rangle + (0.401826 + 0.628144i)|2\rangle,
F_1 = |\varphi_{21}\rangle\langle\varphi_{21}|,
                                                        |\varphi_{21}\rangle = 0.704822|0\rangle + (0.050276 - 0.044858i)|1\rangle + (-0.676460 + 0.202702i)|2\rangle,
F_2 = I - |\varphi_{22}\rangle\langle\varphi_{22}|,
                                                        |\varphi_{22}\rangle = 0.279921|0\rangle + (-0.406294 + 0.685472i)|1\rangle + (0.534341 + 0.034308i)|2\rangle,
F_3 = I - |\varphi_{23}\rangle\langle\varphi_{23}|,
                                                        |\varphi_{23}\rangle = 0.580814|0\rangle + (0.563163 + 0.064963i)|1\rangle + (0.561359 - 0.161735i)|2\rangle,
F_4 = I - |\varphi_{24}\rangle\langle\varphi_{24}|,
                                                        |\varphi_{24}\rangle = 0.522791|0\rangle + (-0.366663 - 0.240466i)|1\rangle + (-0.161766 - 0.712921i)|2\rangle,
F_5 = I - |\varphi_{25}\rangle\langle\varphi_{25}|,
                                                        |\varphi_{25}\rangle = 0.575083|0\rangle + (0.352241 + 0.118045i)|1\rangle + (-0.170766 - 0.708598i)|2\rangle
E_1 = |\varphi_{11}\rangle\langle\varphi_{11}|,
                                                        |\varphi_{11}\rangle = 0.589845|0\rangle + (0.252414 - 0.592962i)|1\rangle + (-0.067286 + 0.481911i)|2\rangle,
                                                        |\varphi_{12}\rangle = 0.571429|0\rangle + (-0.328221 - 0.214531i)|1\rangle + (0.352103 + 0.629079i)|2\rangle,
E_2 = |\varphi_{12}\rangle\langle\varphi_{12}|,
E_3 = I - |\varphi_{13}\rangle\langle\varphi_{13}|,
                                                        |\varphi_{13}\rangle = 0.789596|0\rangle + (0.397845 + 0.124284i)|1\rangle + (0.373987 + 0.250887i)|2\rangle,
E_4 = I - |\varphi_{14}\rangle\langle\varphi_{14}|,
                                                        |\varphi_{14}\rangle = 0.588353|0\rangle + (-0.068306 - 0.217513i)|1\rangle + (-0.748446 + 0.204184i)|2\rangle,
F_1 = |\varphi_{21}\rangle\langle\varphi_{21}|,
                                                        |\varphi_{21}\rangle = 0.500028|0\rangle + (-0.062398 + 0.498087i)|1\rangle + (-0.351826 - 0.611724i)|2\rangle,
F_2 = |\varphi_{22}\rangle\langle\varphi_{22}|,
                                                        |\varphi_{22}\rangle = 0.416357|0\rangle + (-0.421270 + 0.580072i)|1\rangle + (0.375055 - 0.414762i)|2\rangle,
                                                        |\varphi_{23}\rangle = 0.555120|0\rangle + (-0.275989 - 0.322007i)|1\rangle + (0.606921 - 0.378986i)|2\rangle,
F_3 = |\varphi_{23}\rangle\langle\varphi_{23}|,
F_4 = I - |\varphi_{24}\rangle\langle\varphi_{24}|,
                                                        |\varphi_{24}\rangle = 0.771642|0\rangle + (0.389862 + 0.263652i)|1\rangle + (0.160470 - 0.396628i)|2\rangle,
F_5 = I - |\varphi_{25}\rangle\langle\varphi_{25}|,
                                                        |\varphi_{25}\rangle = 0.759855|0\rangle + (0.022187 + 0.015402i)|1\rangle + (0.430543 - 0.486336i)|2\rangle
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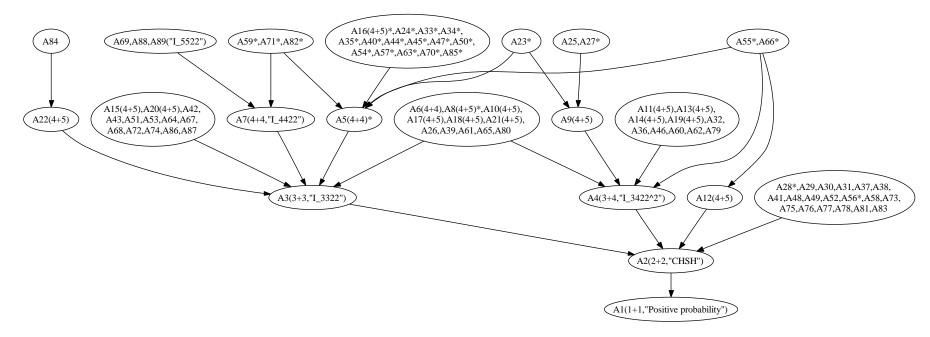


FIG. 1: Inclusion relation among 89 Bell inequalities, with at most 5 measurements per party, obtained by triangular elimination from facets of CUT_9^{\square} . An asterisk (*) on the right of the serial number indicates that the inequality is relevant to the CHSH inequality for $3 \otimes 3$ isotropic states and that it is a candidate for being relevant to I_{3322} .